

09/898,941

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.26

1.26

FILE 'REGISTRY' ENTERED AT 16:56:59 ON 09 NOV 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4

DICTIONARY FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

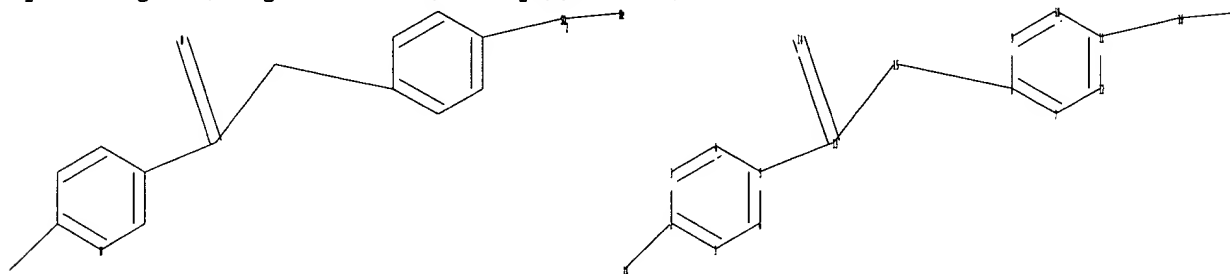
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\rkc941.str



```

chain nodes :
13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-18 5-13 8-15 11-16 13-14 13-15 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
13-14
exact bonds :
2-18 5-13 8-15 11-16 13-15 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

```

```
L1      STRUCTURE UPLOADED
```

```

=> s k1 ful
L2      19574 K1

```

```

=> d 1 fhitr
'FHITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

```

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

```

REG      - RN
SAM      - Index Name, MF, and structure - no RN
FIDE     - All substance data, except sequence data
IDE      - FIDE, but only 50 names
SQIDE    - IDE, plus sequence data
SQIDE3   - Same as SQIDE, but 3-letter amino acid codes are used
SQD      - Protein sequence data, includes RN
SQD3     - Same as SQD, but 3-letter amino acid codes are used
SQN      - Protein sequence name information, includes RN

CALC     - Table of calculated properties
EPROP    - Table of experimental properties
PROP     - EPROP and CALC

```

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

```

ABS      -- Abstract
APPS     -- Application and Priority Information
BIB      -- CA Accession Number, plus Bibliographic Data

```

CAN -- CA Accession Number
 CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
 IND -- Index Data
 IPC -- International Patent Classification
 PATS -- PI, SO
 STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
 IBIB -- BIB, indented, with text labels
 ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
 HELP FORMATS -- To see detailed descriptions of the predefined formats.
 ENTER DISPLAY FORMAT (IDE):d 1
 'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
 SAM - Index Name, MF, and structure - no RN
 FIDE - All substance data, except sequence data
 IDE - FIDE, but only 50 names
 SQIDE - IDE, plus sequence data
 SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
 SQD - Protein sequence data, includes RN
 SQD3 - Same as SQD, but 3-letter amino acid codes are used
 SQN - Protein sequence name information, includes RN

 CALC - Table of calculated properties
 EPROP - Table of experimental properties
 PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
 APPS -- Application and Priority Information
 BIB -- CA Accession Number, plus Bibliographic Data
 CAN -- CA Accession Number
 CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data
 IPC -- International Patent Classification
 PATS -- PI, SO
 STD -- BIB, IPC, and NCL

 IABS -- ABS, indented, with text labels
 IBIB -- BIB, indented, with text labels
 ISTD -- STD format, indented

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
 HELP FORMATS -- To see detailed descriptions of the predefined formats.
 ENTER DISPLAY FORMAT (IDE):
 ENTER DISPLAY FORMAT (IDE):ide

L2 ANSWER 1 OF 19574 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 865506-50-9 REGISTRY
 ED Entered STN: 18 Oct 2005
 CN Cytidyltransferase, acylneuraminate (Escherichia coli strain K1 RS218 gene neuA) (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 29: PN: WO2005090552 FIGURE: 4 claimed sequence
 FS PROTEIN SEQUENCE
 MF Unspecified
 CI MAN
 SR CA
 LC STN Files: CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 *** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 1000

L2 ANSWER 1000 OF 19574 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 754259-45-5 REGISTRY
 ED Entered STN: 30 Sep 2004
 CN DNA (Gossypium hirsutum clone LIB3585-038-P1-K1-G7 EST (expressed sequence tag)) (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 1502: PN: US20040181830 SEQID: 1502 claimed DNA
 FS NUCLEIC ACID SEQUENCE
 MF Unspecified
 CI MAN

SR CA
LC STN Files: CA, CAPLUS, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
*** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 1500

L2 ANSWER 1500 OF 19574 REGISTRY COPYRIGHT 2005 ACS on STN
RN 753049-21-7 REGISTRY
ED Entered STN: 28 Sep 2004
CN Protein (sorghum clone LIB3480-049-P1-K1-B8.pep fragment) (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN 979: PN: US20040172684 SEQID: 50979 claimed protein
FS PROTEIN SEQUENCE
MF Unspecified
CI MAN
SR CA
LC STN Files: CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
*** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

| | | |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 11.41 | 12.67 |

FILE 'CAPLUS' ENTERED AT 16:58:57 ON 09 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 9 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 8 Nov 2005 (20051108/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 12

L3 27567 L2

=> d fhitstr

L3 ANSWER 1 OF 27567 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 7681-11-0, Potassium iodide
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (synergistic topically applied personal hygiene product)
 RN 7681-11-0 CAPLUS
 CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I-K

=> d 22000 fhitstr

L3 ANSWER 22000 OF 27567 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 7681-11-0, properties
 RL: PRP (Properties)
 (electron emission from, secondary)
 RN 7681-11-0 CAPLUS
 CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I-K

=> dis his

(FILE 'HOME' ENTERED AT 16:53:21 ON 09 NOV 2005)

FILE 'REGISTRY' ENTERED AT 16:56:59 ON 09 NOV 2005

L1 STRUCTURE UPLOADED
 L2 19574 S K1 FUL

FILE 'CAPLUS' ENTERED AT 16:58:57 ON 09 NOV 2005

L3 27567 S L2

=> s l3 and acetonitrile

76750 ACETONITRILE
 L4 255 L3 AND ACETONITRILE

=> d

L4 ANSWER 1 OF 255 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2005:467929 CAPLUS
 DN 143:7613
 TI Simple preparation of zaltoprofen from diphenyl sulfide derivatives
 IN Nakada, Yoshitaka
 PA Ohara Pharmaceutical Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-----------------|------|----------|-----------------|----------|
| PI | JP 2005139120 | A2 | 20050602 | JP 2003-377810 | 20031107 |
| PRAI | JP 2003-377810 | | 20031107 | | |
| OS | MARPAT 143:7613 | | | | |

=> d hitstr

L4 ANSWER 1 OF 255 CAPLUS COPYRIGHT 2005 ACS on STN

IT 7681-11-0, Potassium iodide, uses

RL: CAT (Catalyst use); USES (Uses)

(preparation of zaltoprofen from alkyl acetyl(phenylthiophenyl)acetates with 4 steps)

RN 7681-11-0 CAPLUS

CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I-K

=> d 100 hitstr

L4 ANSWER 100 OF 255 CAPLUS COPYRIGHT 2005 ACS on STN

IT 7681-11-0, Potassium iodide (KI), uses

RL: NUU (Other use, unclassified); USES (Uses)

(indirect electrolytic oxidative coupling reaction of some activated methylene compds. studied using KI-NaI as indirect electrolyte and acetone as solvent)

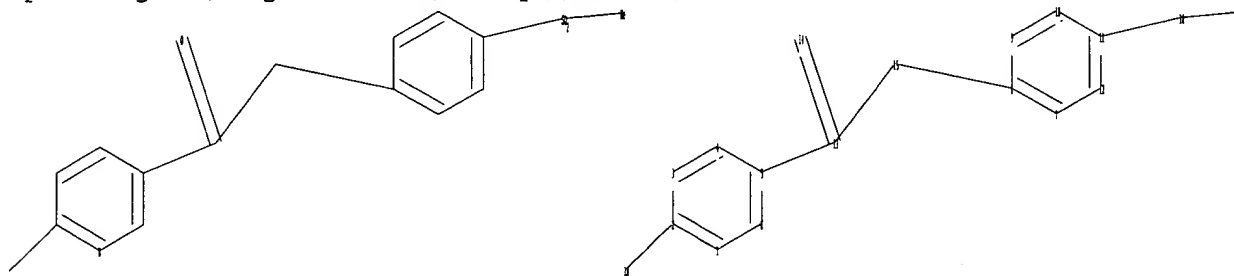
RN 7681-11-0 CAPLUS

CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I-K

=>

Uploading C:\Program Files\Stnexp\Queries\rkc941.str



```

chain nodes :
13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-18 5-13 8-15 11-16 13-14 13-15 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
13-14
exact bonds :
2-18 5-13 8-15 11-16 13-15 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

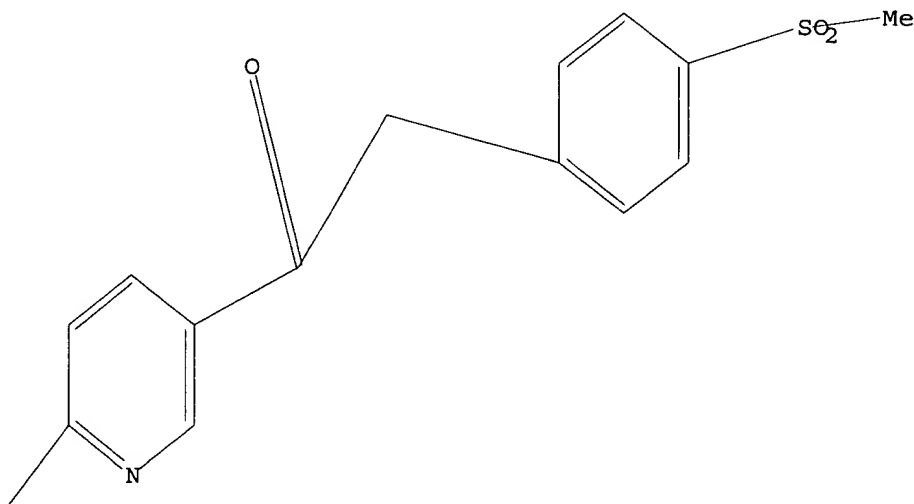
```

L5 STRUCTURE UPLOADED

```

=> d
L5 HAS NO ANSWERS
L5                STR

```



Structure attributes must be viewed using STN Express query preparation.

```

=> fil reg
COST IN U.S. DOLLARS
FULL ESTIMATED COST

```

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 14.40 | 27.07 |

FILE 'REGISTRY' ENTERED AT 17:02:03 ON 09 NOV 2005

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STRUCTURE FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4
 DICTIONARY FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS
 for details.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> s l5

SAMPLE SEARCH INITIATED 17:02:06 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 0 TO 0
 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s l5 ful

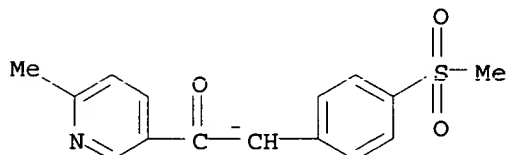
FULL SEARCH INITIATED 17:02:13 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS 4 ANSWERS
 SEARCH TIME: 00.00.01

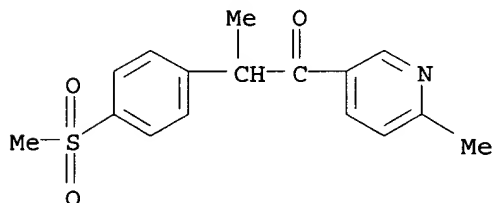
L7 4 SEA SSS FUL L5

=> d 1-4

L7 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 788151-35-9 REGISTRY
 ED Entered STN: 25 Nov 2004
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-)
 (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C15 H14 N O3 S
 CI COM
 SR CA



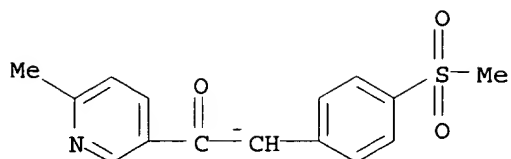
L7 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 452332-13-7 REGISTRY
 ED Entered STN: 18 Sep 2002
 CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C16 H17 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 452332-12-6 REGISTRY
 ED Entered STN: 18 Sep 2002
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-),
 potassium (9CI) (CA INDEX NAME)
 MF C15 H14 N O3 S . K
 SR CA
 LC STN Files: CA, CAPLUS
 CRN (788151-35-9)



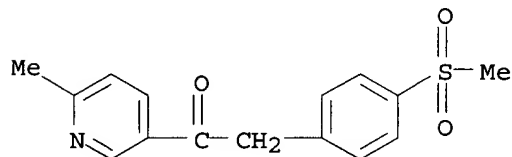
● K⁺

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 221615-75-4 REGISTRY
ED Entered STN: 25 Apr 1999
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
FS 3D CONCORD
MF C15 H15 N O3 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, PS, TOXCENTER, USPAT2,
USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 168.69 | 195.76 |

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:02:26 ON 09 NOV 2005
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FILE COVERS 1907 - 9 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 8 Nov 2005 (20051108/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 17

L8 16 L7

=> d 1-16 fhitstr

L8 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

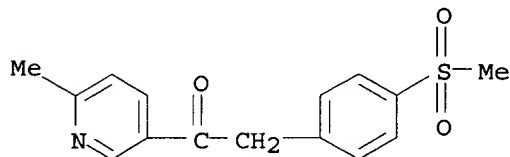
IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

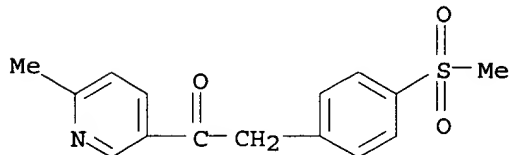
IT 221615-75-4

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)

(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)

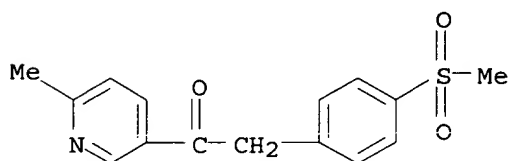
RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

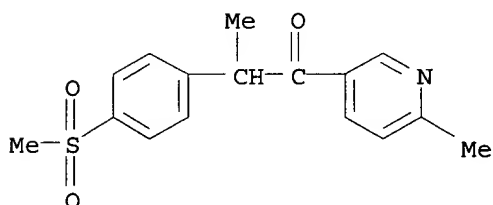


L8 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

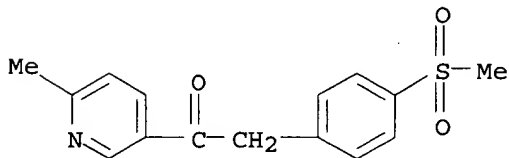
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of
 resp. methylthiophenyl derivative)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl] - (9CI)
 (CA INDEX NAME)



L8 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 452332-13-7
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
 nonpreparative)
 (LC-mass spectra of)
 RN 452332-13-7 CAPLUS
 CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl] - (9CI)
 (CA INDEX NAME)

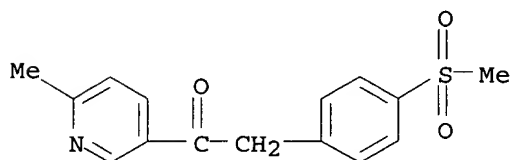


L8 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 221615-75-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (treatment of cancer with prostate specific antigen (PSA) conjugate and
 NSAID compound)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl] - (9CI)
 (CA INDEX NAME)

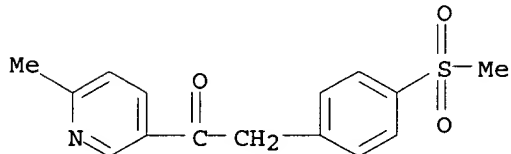


L8 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

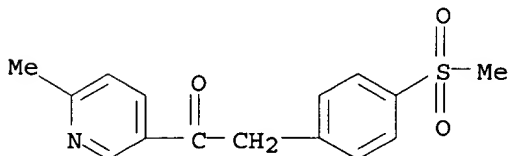
IT 221615-75-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and
 process for synthesis)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



L8 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



L8 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 221615-75-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the preparation of intermediates useful in the synthesis of diarylpyridines)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



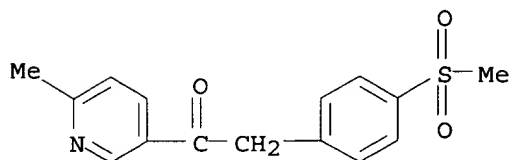
L8 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

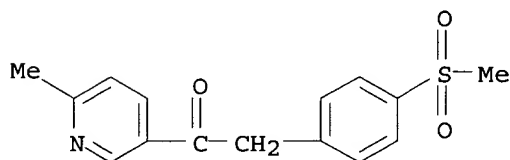
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

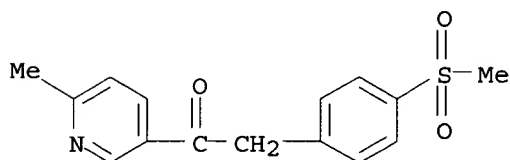
IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

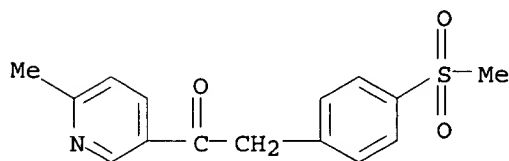
IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

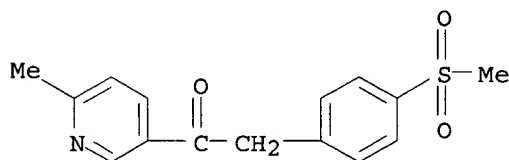
L8 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

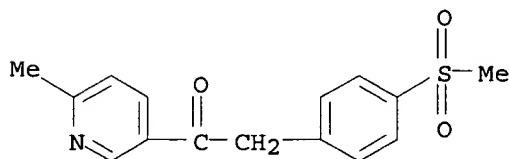
L8 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

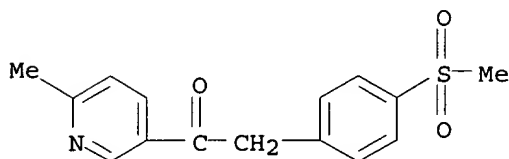
L8 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone

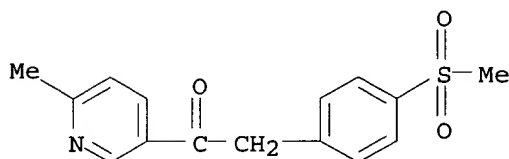
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of arylpyridine COX-2 inhibitors by
cyclocondensation of iminium salts with ketones)

RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



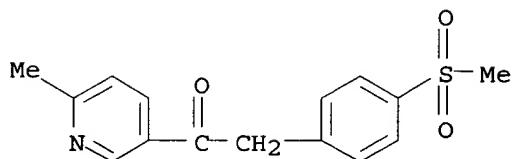
L8 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



=> d 1-16 bib abs fhitr

L8 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:406839 CAPLUS
Correction of: 2005:155216
DN 143:248209
Correction of: 142:197768
TI Product class 1: pyridines
AU Spitzner, D.
CS Germany
SO Science of Synthesis (2005), 15, 11-284
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review of methods to prepare pyridines, pyridine-1-oxides, and pyridinium salts. Methods include cyclization, ring transformations, aromatization and substituent modification.
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:586395 CAPLUS

DN 140:117549

TI Development and validation of an HPLC method for the impurity and quantitative analysis of etoricoxib

AU Hartman, Robert; Abraham, Ahmed; Clausen, Andrew; Mao, Bing; Crocker, Louis S.; Ge, Zhihong

CS Analytical Research, Merck Research Laboratories, Rahway, NJ, 07065-0914, USA

SO Journal of Liquid Chromatography & Related Technologies (2003), 26(15), 2551-2566

CODEN: JLCTFC; ISSN: 1082-6076

PB Marcel Dekker, Inc.

DT Journal

LA English

AB Etoricoxib (5-chloro-6'-methyl-3[4-(methanesulfonyl)phenyl]-2,3'-bipyridine) is a highly active and selective cyclo-oxygenase II inhibitor. A single, stability-indicating HPLC method was developed and validated for both the impurity and quant. anal. of etoricoxib. Method development incorporated the optimization of stationary phase, pH, temperature, and mobile phase composition for the resolution of 13 process impurities and 3 major degradation

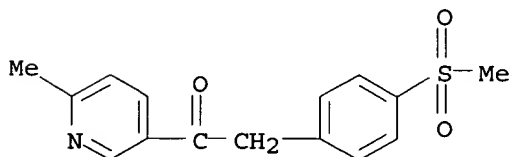
products. Further optimization of pH and mobile phase composition was aided by the use of DryLab, a computer-based simulation program. The stability-indicating capability of the method was proven through the identification of photolytic and oxidative decomposition products. Method validation produced excellent results for linearity, precision, limit of quantitation and limit of detection, specificity, accuracy, recovery, and robustness. The identities of etoricoxib decomposition products were confirmed by UV, LC/MS, and NMR spectra.

IT 221615-75-4

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)

RN 221615-75-4 CAPLUS

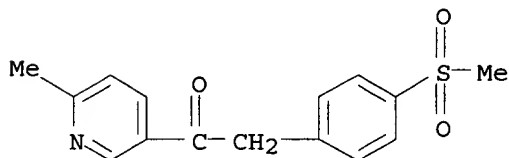
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

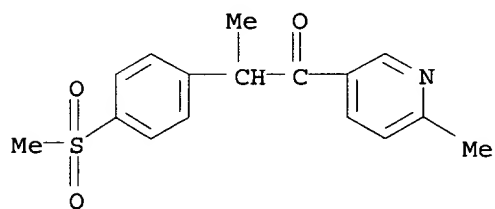
L8 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:491189 CAPLUS
DN 139:70705
TI Production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation
of the respective methylthiophenyl derivative
IN Cannata, Vincenzo; Soriato, Giorgio; Verzini, Massimo
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2003051843 | A1 | 20030626 | WO 2002-EP14115 | 20021212 |
| | W: CN, CZ, HU, IL, IN, US | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR | | | | |
| | EP 1492770 | A1 | 20050105 | EP 2002-795165 | 20021212 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK | | | | |
| | US 2005165238 | A1 | 20050728 | US 2003-499321 | 20021212 |
| PRAI | IT 2001-MI2692 | A | 20011219 | | |
| | WO 2002-EP14115 | W | 20021212 | | |
| OS | CASREACT 139:70705 | | | | |
| AB | A process for production of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone is carried out by oxidation of 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone with an oxidant in the presence of an acid, the oxidant being a mixture of peracetic acid and hydrogen peroxide, and the acid being methanesulfonic acid. The product is useful as an intermediate in production of cyclooxygenase 2 (COX 2) inhibitors. Thus, the title compound was produced in 88.6% yield by mixing 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone (30), acetic acid (45), methanesulfonic acid (13.6), adding Oxystromg (65% peracetic acid) (28.1 kg) at 35°, and reacting the mixture at 35° for 3-4 h. | | | | |
| IT | 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone | | | | |
| | RL: IMF (Industrial manufacture); PREP (Preparation) (production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative) | | | | |
| RN | 221615-75-4 CAPLUS | | | | |
| CN | Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME) | | | | |



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

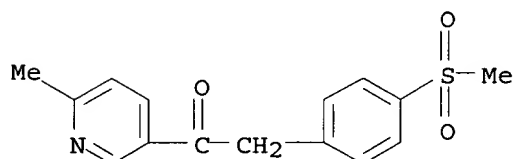
L8 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:434902 CAPLUS
 DN 137:210102
 TI Development of a derivatization method, coupled with reverse phase HPLC, for monitoring the formation of an enolate intermediate
 AU Abraham, A.; Hartman, R.; Ge, Z.; Mao, B.; Marcoux, J.
 CS Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
 SO Journal of Liquid Chromatography & Related Technologies (2002), 25(7), 1049-1062
 CODEN: JLCTFC; ISSN: 1082-6076
 PB Marcel Dekker, Inc.
 DT Journal
 LA English
 AB A sensitive liquid chromatog. method was developed to monitor the formation of an enolate intermediate in a synthetic route to Etoricoxib, a drug candidate for the treatment of arthritis. The method requires the derivatization of the enolate with Me iodide to form a stable methylketosulfone derivative followed by reverse phase HPLC anal. Parameters affecting the derivatization, including the nature of derivatizing agent, reaction solvent, amount of derivatizing agent, reaction time, reaction temperature, and amount of excess base in the reaction were studied. The derivatization reaction gave selective C-alkylation. The linear range of the chromatog. method for the determination of the starting material, ketosulfone, and the derivative, methylketosulfone, was determined Finally, the accuracy of the method was established based on recovery expts.
 IT 452332-13-7
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (LC-mass spectra of)
 RN 452332-13-7 CAPLUS
 CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:276519 CAPLUS
 DN 136:310188
 TI Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound
 IN Heimbrook, David C.; Yao, Siu-long
 PA USA
 SO U.S. Pat. Appl. Publ., 129 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | US 2002042375 | A1 | 20020411 | US 2001-896245 | 20010629 |
| PRAI | US 2000-216217P | P | 20000705 | | |
| OS | MARPAT 136:310188 | | | | |
| AB | The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg = cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given). | | | | |
| IT | 221615-75-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound) | | | | |
| RN | 221615-75-4 CAPLUS | | | | |
| CN | Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME) | | | | |



L8 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:886073 CAPLUS
DN 136:11103
TI 5-chloro-3-(4-methanesulfonylphenyl)-6'-methyl- [2,3']bipyridinyl in pure crystalline form and process for synthesis
IN Crocker, Louis S.; Davies, Ian W.; Osifchin, Richard G.; Kotliar, Andrew
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| PI | WO 2001092230 | A1 | 20011206 | WO 2001-US16566 | 20010522 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2410234 | AA | 20011206 | CA 2001-2410234 | 20010522 |
| | EP 1296951 | A1 | 20030402 | EP 2001-939267 | 20010522 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

| | | | | |
|---------------|----|----------|----------------|----------|
| JP 2004501116 | T2 | 20040115 | JP 2002-500844 | 20010522 |
| JP 3665053 | B2 | 20050629 | | |
| NZ 522394 | A | 20040528 | NZ 2001-522394 | 20010522 |
| EE 200200655 | A | 20040816 | EE 2002-655 | 20010522 |
| BR 2001011140 | A | 20050111 | BR 2001-11140 | 20010522 |
| BG 107237 | A | 20030530 | BG 2002-107237 | 20021031 |
| ZA 2002009558 | A | 20031028 | ZA 2002-9558 | 20021125 |
| JP 2005047927 | A2 | 20050224 | JP 2004-263913 | 20040910 |

PRAI US 2000-208017P P 20000526

JP 2002-500844 A3 20010522

WO 2001-US16566 W 20010522

AB This invention encompasses the form V polymorph of the title composition which is useful in the treatment of cyclooxygenase-2 mediated diseases. The invention encompasses certain pharmaceutical compns. for treatment of cyclooxygenase-2 mediated diseases comprising the Form V polymorph of the title composition. The invention also encompasses a process for synthesizing the form V polymorph of the title composition. A mixture of the title composition and

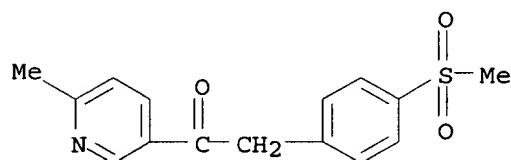
iso-Pr acetate was heated at 55°, then was cooled to ambient temperature and the solids were isolated by filtration. The solids were washed with iso-Pr acetate and dried in vacuo to give the form V polymorph as a colorless solid in about 87% yield.

IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300685 CAPLUS

DN 134:311114

TI Process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone

IN Cannata, Vincenzo; Rossato, Roberto

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 9 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| | ----- | --- | ---- | ----- | ----- |
| PI | WO 2001029004 | A1 | 20010426 | WO 2000-EP9995 | 20001011 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, | | | | |

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
 LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

IT 99MI2156 A1 20010416 IT 1999-MI2156 19991015

PRAI IT 1999-MI2156 A 19991015

OS CASREACT 134:311114

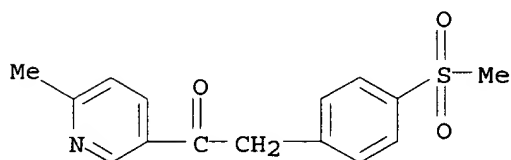
AB A process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone (I) into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone, a pharmaceutical intermediate (no data), without the formation of N-oxide byproduct, consists of reacting I with an oxidant (e.g., a mixture of peracetic acid and hydrogen peroxide) in the presence of a catalyst (e.g., sodium tungstate) and an acid (e.g. methanesulfonic acid).

IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300684 CAPLUS

DN 134:295751

TI Process for the preparation of intermediates useful in the synthesis of diarylpyridines

IN Allegrini, Pietro; Verzini, Massimo

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DT Patent

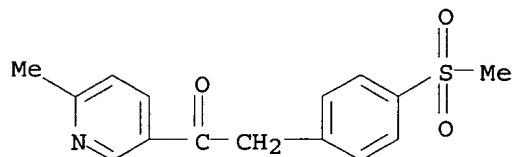
LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|---|----------|-----------------|----------|
| PI | WO 2001029003 | A1 | 20010426 | WO 2000-EP9994 | 20001011 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, | | | |

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

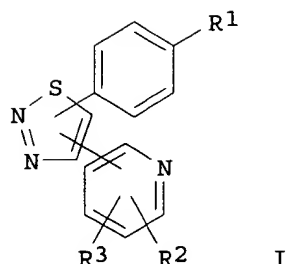
IT 99MI2157 A1 20010416 IT 1999-MI2157 19991015
 PRAI IT 1999-MI2157 A 19991015
 OS CASREACT 134:295751; MARPAT 134:295751
 AB This process is used to prepare intermediates useful in the synthesis of
 diarylpyridines having COX-2 inhibitor activity. E.g., reaction of
 6-methylnicotinic acid Me ester with (4-methylthiophenyl)acetonitrile gave
 3-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)-3-oxopropionitrile
 hydrochloride. Acid hydrolysis and decarboxylation of the latter gave
 1-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)ethanone.
 IT 221615-75-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the preparation of intermediates useful in the synthesis of
 diarylpyridines)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:185752 CAPLUS
 DN 134:222716
 TI 1,2,3-Thiadiazoles and their use as COX-2 inhibitors
 IN Lau, Cheuk K.; Li, Chun Sing; Therien, Michel; Gauthier, Jacques Y.
 PA Merck Frosst Canada & Co., Can.
 SO PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2001017996 | A1 | 20010315 | WO 2000-CA1040 | 20000907 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| PRAI US 1999-152746P | P | 19990908 | | |
| OS MARPAT 134:222716 | | | | |
| GI | | | | |

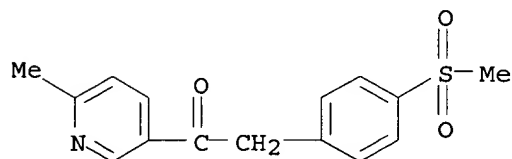


AB Title compds. I [R1 = SO₂Me, S(O)NHMe, S(O)NHNH₂, P(O)MeOH, etc.; R2, R3 = H, halo, alkoxy, alkyl, CN, etc.] were prepared Thus, 4-(6-methyl-3-pyridinyl)-5-[4-(methylsulfonyl)phenyl]-1,2,3-thiadiazole (II) was prepared in 5 steps starting from 6-methylnicotinic acid and N-methoxymethylamine hydrochloride. Oxidation of II with H₂O₂ gave the thiadiazole 3-oxide. Inhibition of COX-2 was determined by measuring the effects on PGE₂ production in whole blood.

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:78362 CAPLUS

DN 134:131435

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone starting from 4-methylthiobenzyl alcohol and 6-methylnicotinate esters.

IN Bessard, Yves; Leresche, James Edward

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2001007410 | A1 | 20010201 | WO 2000-EP6825 | 20000717 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, | | | | |

HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1198455 A1 20020424 EP 2000-951393 20000717
 EP 1198455 B1 20031210

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL

JP 2003505449 T2 20030212 JP 2001-512497 20000717
 AT 256112 E 20031215 AT 2000-951393 20000717
 ES 2207536 T3 20040601 ES 2000-951393 20000717
 US 6566527 B1 20030520 US 2002-30096 20020314
 US 2003088107 A1 20030508 US 2002-283167 20021030
 US 6600046 B2 20030729

PRAI EP 1999-114667 A 19990727
 US 2000-186680P P 20000303
 WO 2000-EP6825 W 20000717
 US 2002-30096 A3 20020314

OS CASREACT 134:131435

AB 1-(6-Methylpyridin-3-yl)-2-[(4-methylsulfonyl)phenyl]ethanone was prepared by (a) treatment of 4-(methylthio)benzyl alc. with hydrochloric acid to give 4-(methylthio)benzyl chloride, (b) treatment of this with an alkali metal cyanide to give 4-(methylthio)phenylacetonitrile, (c) condensation of 4-(methylthio)phenylacetonitrile with a 6-methylnicotinate ester to give 3-[2-(4-methylthiophenyl)-2-cyanoacetyl]-6-methylpyridine, (d) hydrolysis and decarboxylation under acidic conditions to give 3-[2-(4-methylthiophenyl)acetyl]-6-methylpyridine and (e) oxidation

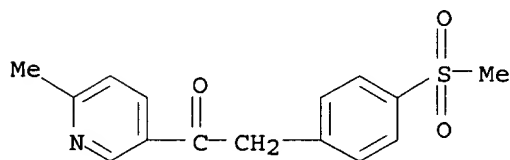
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)

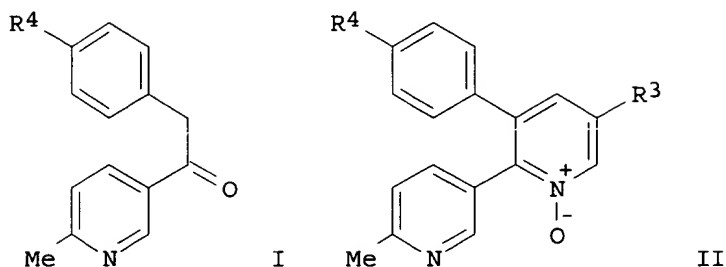


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:897114 CAPLUS
 DN 134:178439
 TI A general [3 + 2 + 1] annulation strategy for the preparation of pyridine N-oxides
 AU Davies, Ian W.; Marcoux, Jean-Francois; Reider, Paul J.
 CS Department of Process Research, Merck & Co. Inc., Rahway, NJ, 07065, USA
 SO Organic Letters (2001), 3(2), 209-211

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 134:178439
 GI



AB Stabilized ketone, aldehyde, and ester enolates, generated from I (R4 = MeSO2, MeS) for example, react with vinamidinium hexafluorophosphate salts and hydroxylamine hydrochloride to give pyridine N-oxides, e.g. II (R3 = Cl, NO2), in 45-85% yields.

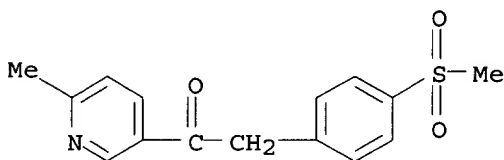
IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:653182 CAPLUS

DN 134:4838

TI A Practical Synthesis of a COX-2-Specific Inhibitor

AU Davies, Ian W.; Marcoux, Jean-Francois; Corley, Edward G.; Journet, Michel; Cai, Dong-Wei; Palucki, Michael; Wu, Jimmy; Larsen, Robert D.; Rossen, Kai; Pye, Philip J.; DiMichele, Lisa; Dormer, Peter; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

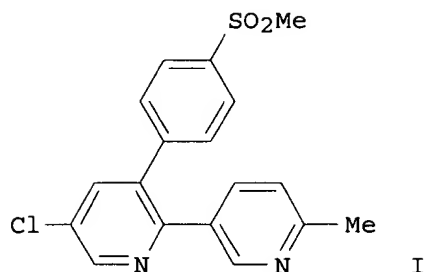
SO Journal of Organic Chemistry (2000), 65(25), 8415-8420

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English
OS CASREACT 134:4838
GI



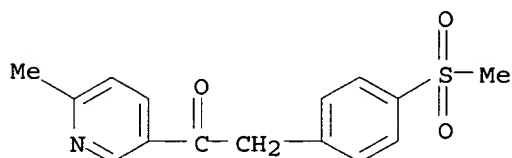
AB A number of synthetic strategies to the Cox-2 specific inhibitor have been described. These studies have led to the identification of a novel pyridine construction using annulation of a ketone using a vinamidinium species and ammonia in 97% assay yield. Three approaches to the synthesis of the ketone are described that allow for its preparation in large quantities in >65% overall yield from Me 6-methylnicotinate.

IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:493518 CAPLUS

DN 133:104966

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.

IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 19 pp.

CODEN: PIXXD2

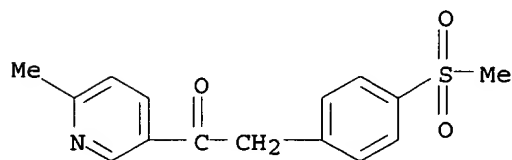
DT Patent

LA German

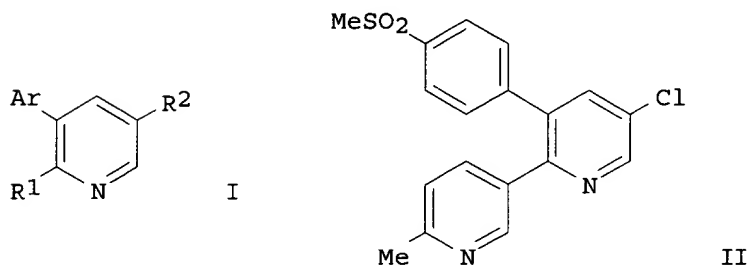
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|----------|-----------------|----------|
| | ----- | --- | ----- | ----- | ----- |
| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |

WO 2000042014 A3 20001207
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2359958 AA 20000720 CA 2000-2359958 20000113
CA 2485739 AA 20000720 CA 2000-2485739 20000113
EP 1159270 A2 20011205 EP 2000-901555 20000113
EP 1159270 B1 20031105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
JP 2003518002 T2 20030603 JP 2000-593582 20000113
AT 253559 E 20031115 AT 2000-901555 20000113
EP 1394149 A1 20040303 EP 2003-24787 20000113
EP 1394149 B1 20050119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY
PT 1159270 T 20040331 PT 2000-901555 20000113
ES 2209807 T3 20040701 ES 2000-901555 20000113
AT 287396 E 20050215 AT 2003-24787 20000113
PT 1394149 T 20050531 PT 2003-24787 20000113
ES 2235138 T3 20050701 ES 2003-3024787 20000113
NO 2001003498 A 20010905 NO 2001-3498 20010713
US 2005159458 A1 20050721 US 2005-29489 20050106
PRAI EP 1999-100590 A 19990114
US 1999-145996P P 19990729
CA 2000-2359958 A3 20000113
EP 2000-901555 A3 20000113
WO 2000-EP240 W 20000113
US 2003-868941 A3 20031104
OS CASREACT 133:104966
AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

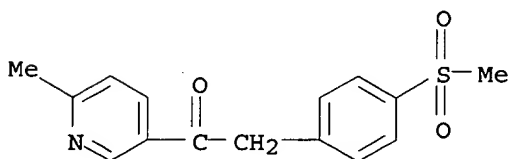


L8 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:443023 CAPLUS
 DN 133:222553
 TI Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines
 AU Marcoux, Jean-Francois; Corley, Edward G.; Rossen, Kai; Pye, Phil; Wu, Jimmy; Robbins, Michael A.; Davies, Ian W.; Larsen, Robert D.; Reider, Paul J.
 CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA
 SO Organic Letters (2000), 2(15), 2339-2341
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 133:222553
 GI



AB α -Aryl ketones react with vinamidinium hexafluorophosphate salts to give access to the corresponding 3-arylpyridines I (Ar = C₆H₄R-4, R = SO₂Me, H, SMe, R₁ = 6-methyl-3-pyridyl, C₆H₄R-4, R₂ = Cl; Ar = C₆H₄SO₂Me-4, R₁ = 6-methyl-3-pyridyl, R₂ = Br, I, CF₃, NO₂, phthalimido; Ar = C₆H₄F-4, R₁ = Me, R₂ = Cl; Ar = Ph, R₁ = H, R₂ = Cl). The annulation reactions proceed in good to excellent yields with vinamidinium salts containing electron-withdrawing groups at the β -position (R₂). The reaction was applied to the preparation of the COX-2 specific inhibitor 5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine (II), as well as a series of analogs.

IT 221615-75-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:708874 CAPLUS
DN 131:322542
TI Process for synthesizing arylpyridine COX-2 inhibitors
IN Corley, Edward G.; Davies, Ian W.; Larsen, Robert D.; Pye, Philip J.;
Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|------------------|----------|
| PI | WO 9955830 | A2 | 19991104 | WO 1999-US8645 | 19990420 |
| | WO 9955830 | A3 | 19991229 | | |
| | W: | | | | |
| | AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2329193 | AA | 19991104 | CA 1999-2329193 | 19990420 |
| | EP 1071745 | A2 | 20010131 | EP 1999-918706 | 19990420 |
| | EP 1071745 | B1 | 20040804 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
| | BR 9909844 | A | 20010403 | BR 1999-9844 | 19990420 |
| | JP 2002513035 | T2 | 20020508 | JP 2000-545976 | 19990420 |
| | JP 3325264 | B2 | 20020917 | | |
| | AU 759469 | B2 | 20030417 | AU 1999-36557 | 19990420 |
| | CZ 292515 | B6 | 20031015 | CZ 2000-3940 | 19990420 |
| | NZ 507597 | A | 20040227 | NZ 1999-507597 | 19990420 |
| | AT 272613 | E | 20040815 | AT 1999-918706 | 19990420 |
| | PT 1071745 | T | 20041130 | PT 1999-918706 | 19990420 |
| | ES 2226378 | T3 | 20050316 | ES 1999-918706 | 19990420 |
| | US 6040319 | A | 20000321 | US 1999-298127 | 19990423 |
| | TW 474934 | B | 20020201 | TW 1999-88106545 | 19990423 |
| | US 6252116 | B1 | 20010626 | US 2000-488774 | 20000121 |
| | HR 2000000722 | A1 | 20010630 | HR 2000-722 | 20001024 |
| | HK 1031399 | A1 | 20041217 | HK 2001-102195 | 20010326 |
| PRAI | US 1998-82888P | P | 19980424 | | |
| | US 1998-85668P | P | 19980515 | | |
| | WO 1999-US8645 | W | 19990420 | | |
| | US 1999-298127 | A3 | 19990423 | | |
| OS | CASREACT 131:322542; MARPAT 131:322542 | | | | |
| GI | | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention encompasses a process and intermediates for preparing compds. I
[R, R', R'' = (un)substituted alkyl, aryl, aralkyl, halo, SOMH, SOM-alkyl,

SOM-aryl, NO₂, (di)(alkyl)amino, SOMNH₂, SOMNH-alkyl, SOMNHCOCF₃, cyano; Y = C, N; m = 0, 1, 2]. I are useful in the treatment of cyclooxygenase-2 mediated diseases (no data), i.e., as analgesics, antipyretics, and antiinflammatories. The method comprises cyclocondensation of an iminium salt II [R₂-R₅ = alkyl, aryl, or aralkyl; X⁻ = suitable counterion] with an aryl ketone III in the presence of a base. The method is designed to give high yields at low temps., and with a reduced number of steps. For instance, the bipyridyl derivative IV was prepared on a 1.65-kg scale by reaction of the iminium salt V with ketone VI in THF in the presence of KOBu-tert, followed by quenching in AcOH/THF, basification with concentrated

aqueous

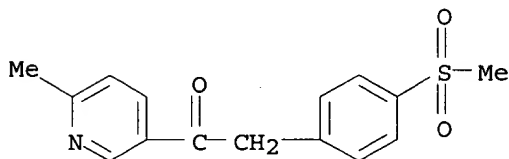
NH₄OH, and refluxing. Prepns. of the salt and ketone intermediates V and VI are described, and a subset of the iminium salt intermediates II are claimed per se.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:222917 CAPLUS

DN 130:252250

TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.

IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 42 pp.

CODEN: PIXXD2

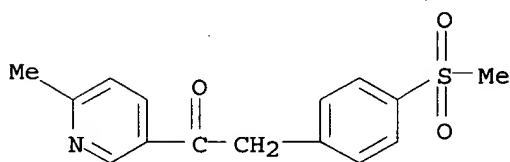
DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|------------|--|----------|-----------------|----------|
| PI | WO 9915503 | A2 | 19990401 | WO 1998-US19788 | 19980922 |
| | WO 9915503 | A3 | 19990520 | | |
| | W: | AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | US 6040450 | A | 20000321 | US 1998-153405 | 19980915 |
| | AU 9895002 | A1 | 19990412 | AU 1998-95002 | 19980922 |
| | EP 1023266 | A2 | 20000802 | EP 1998-948426 | 19980922 |

EP 1023266 B1 20030108
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
BR 9812837 A 20000808 BR 1998-12837 19980922
JP 2001517654 T2 20011009 JP 2000-512812 19980922
JP 3325263 B2 20020917
AT 230726 E 20030115 AT 1998-948426 19980922
ES 2189251 T3 20030701 ES 1998-948426 19980922
CN 1134414 B 20040114 CN 1998-811147 19980922
SK 283811 B6 20040203 SK 2000-422 19980922
US 6204387 B1 20010320 US 2000-509230 20000323
US 6369275 B1 20020409 US 2000-715736 20001117
HK 1029343 A1 20030502 HK 2001-100155 20010106
PRAI US 1997-60680P P 19970925
GB 1998-6419 A 19980325
WO 1998-US19788 W 19980922
US 2000-509230 A3 20000323
OS CASREACT 130:252250; MARPAT 130:252250
AB P-(ArCOCH₂)C₆H₄SO₂R₁ (R₁ = Me, NH₂, NHCOCF₃, NHMe; Ar = mono-, di-, or trisubstituted Ph, pyridyl, N-oxide thereof), were prepared by reaction of p-MeSC₆H₄CH₂MgX (X = Cl, Br, F, iodo) with ArCONMe₂ (Ar as above) to give p-(ArCOCH₂)C₆H₄SMe followed by oxidation of the latter. Thus, the Grignard reagent from p-MeSC₆H₄CH₂Cl in PhMe/THF was added to a -20° solution of 6-methylnicotinic acid N-methyl-N-methoxyamide (preparation given) in PhMe over 30 min. followed by 1 h aging to give 76% 2-methyl-5-(4-methylthiophenylacetyl)pyridine. The latter in MeOH/H₂SO₄ at 55° was treated with aqueous Na tungstate and then with H₂O₂ over 1 h to give 82.5% 2-methyl-5-(4-methylsulfonylphenylacetyl)pyridine. The latter reacted with 3-amino-2-chloroacrolein (preparation given) to give 65% 5-chloro-2-(2-methylpyrid-5-yl)-3-(4-methylsulfonylphenyl)pyridine.
IT 221615-75-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



=>

=>

Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

122.43

318.19

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | -11.68 | -11.68 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 17:11:31 ON 09 NOV 2005

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptaul29rc

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 17:13:09 ON 09 NOV 2005
FILE 'CAPLUS' ENTERED AT 17:13:09 ON 09 NOV 2005
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 122.43 | 318.19 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | -11.68 | -11.68 |

=> dis his

(FILE 'HOME' ENTERED AT 16:53:21 ON 09 NOV 2005)

FILE 'REGISTRY' ENTERED AT 16:56:59 ON 09 NOV 2005

L1 STRUCTURE UPLOADED
L2 19574 S K1 FUL

FILE 'CAPLUS' ENTERED AT 16:58:57 ON 09 NOV 2005

L3 27567 S L2
L4 255 S L3 AND ACETONITRILE
L5 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 17:02:03 ON 09 NOV 2005

L6 0 S L5
L7 4 S L5 FUL

FILE 'CAPLUS' ENTERED AT 17:02:26 ON 09 NOV 2005

L8 16 S L7

=> d l8 16 bib

L8 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:222917 CAPLUS
DN 130:252250
TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.
IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|----------|
| PI | WO 9915503 | A2 | 19990401 | WO 1998-US19788 | 19980922 |
| | WO 9915503 | A3 | 19990520 | | |
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| | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | US 6040450 | A | 20000321 | US 1998-153405 | 19980915 |
| | AU 9895002 | A1 | 19990412 | AU 1998-95002 | 19980922 |
| | EP 1023266 | A2 | 20000802 | EP 1998-948426 | 19980922 |
| | EP 1023266 | B1 | 20030108 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI | | | | |
| | BR 9812837 | A | 20000808 | BR 1998-12837 | 19980922 |
| | JP 2001517654 | T2 | 20011009 | JP 2000-512812 | 19980922 |
| | JP 3325263 | B2 | 20020917 | | |
| | AT 230726 | E | 20030115 | AT 1998-948426 | 19980922 |
| | ES 2189251 | T3 | 20030701 | ES 1998-948426 | 19980922 |
| | CN 1134414 | B | 20040114 | CN 1998-811147 | 19980922 |
| | SK 283811 | B6 | 20040203 | SK 2000-422 | 19980922 |
| | US 6204387 | B1 | 20010320 | US 2000-509230 | 20000323 |
| | US 6369275 | B1 | 20020409 | US 2000-715736 | 20001117 |
| | HK 1029343 | A1 | 20030502 | HK 2001-100155 | 20010106 |
| PRAI | US 1997-60680P | P | 19970925 | | |
| | GB 1998-6419 | A | 19980325 | | |
| | WO 1998-US19788 | W | 19980922 | | |
| | US 2000-509230 | A3 | 20000323 | | |
| OS | CASREACT 130:252250; MARPAT 130:252250 | | | | |

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

123.98

319.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-11.68

-11.68

FILE 'STNGUIDE' ENTERED AT 17:13:45 ON 09 NOV 2005

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Nov 4, 2005 (20051104/UP).

=>

=>

Executing the logoff script...

=> LOG H

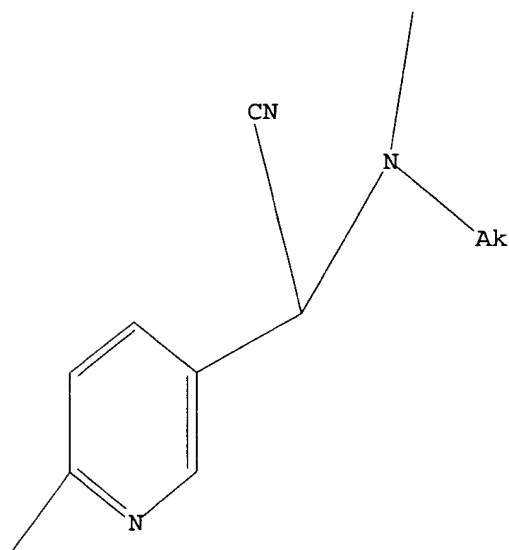
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| CA SUBSCRIBER PRICE | 0.00 | -11.68 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 17:14:10 ON 09 NOV 2005

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 15:41:27 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 72 TO ITERATE

100.0% PROCESSED 72 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L2 1 SEA SSS FUL L1

=>

=> d

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

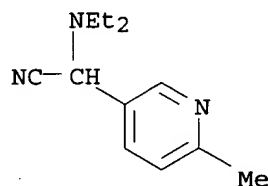
RN 283167-57-7 REGISTRY

ED Entered STN: 04 Aug 2000

CN 3-Pyridineacetonitrile, α -(diethylamino)-6-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H17 N3
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 163.17 | 163.38 |

FILE 'CAPLUS' ENTERED AT 15:41:36 ON 10 NOV 2005
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FILE COVERS 1907 - 10 Nov 2005 VOL 143 ISS 20
 FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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<http://www.cas.org/infopolicy.html>

=> s l2
 L3 1 L2

=> d fbib abs fhitr

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:493518 CAPLUS
 DN 133:104966
 TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethane.

IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward;
 Proplesch, Ralf; Roduit, Jean-Paul
 PA Lonza A.-G., Switz.; Merck & Co., Inc.
 SO PCT Int. Appl., 19 pp.
 CODEN: PIXXD2

DT Patent
 LA German

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|---|----------|-----------------|-----------------|-------------|
| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |
| | WO 2000042014 | A3 | 20001207 | | |
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| | IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, | | | | |
| | MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, | | | | |
| | SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, | | | | |
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| | RW: | | | | |
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| | | | | EP 1999-100590 | A 19990114 |
| | | | | US 1999-145996P | P 19990729 |
| CA 2359958 | AA | 20000720 | CA 2000-2359958 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |
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| | | | CA 2000-2359958 | A3 20000113 | |
| EP 1159270 | A2 | 20011205 | EP 2000-901555 | | 20000113 |
| EP 1159270 | B1 | 20031105 | | | |
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| | IE, SI, LT, LV, FI, RO | | | | |
| | | | | EP 1999-100590 | A 19990114 |
| | | | | US 1999-145996P | P 19990729 |
| | | | | WO 2000-EP240 | W 20000113 |
| JP 2003518002 | T2 | 20030603 | JP 2000-593582 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |
| | | | US 1999-145996P | P 19990729 | |
| | | | WO 2000-EP240 | W 20000113 | |
| AT 253559 | E | 20031115 | AT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |
| | | | US 1999-145996P | P 19990729 | |
| | | | WO 2000-EP240 | W 20000113 | |
| EP 1394149 | A1 | 20040303 | EP 2003-24787 | | 20000113 |
| EP 1394149 | B1 | 20050119 | | | |
| | R: | | | | |
| | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |
| | IE, FI, CY | | | | |
| | | | | EP 1999-100590 | A 19990114 |
| | | | | EP 2000-901555 | A3 20000113 |
| PT 1159270 | T | 20040331 | PT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |
| | | | US 1999-145996P | P 19990729 | |
| ES 2209807 | T3 | 20040701 | ES 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |
| | | | US 1999-145996P | P 19990729 | |
| AT 287396 | E | 20050215 | AT 2003-24787 | | 20000113 |
| | | | EP 1999-100590 | A 19990114 | |

STRUCTURE FILE UPDATES: 8 NOV 2005 HIGHEST RN 866995-49-5
 DICTIONARY FILE UPDATES: 8 NOV 2005 HIGHEST RN 866995-49-5

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 conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
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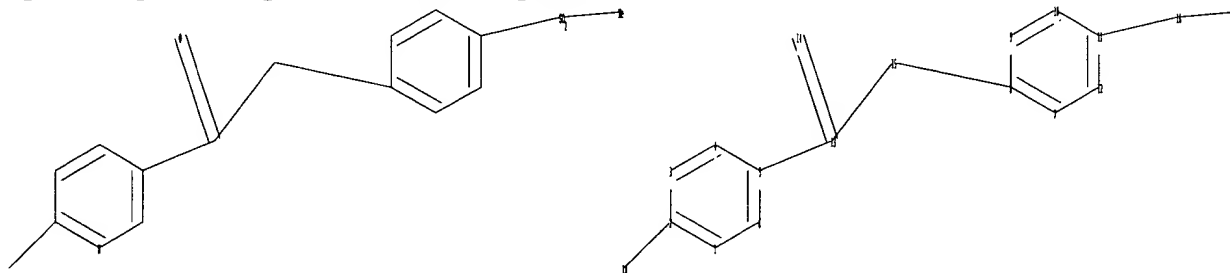
Structure search iteration limits have been increased. See HELP SLIMITS
 for details.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\rkc941.str



chain nodes :

13 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

2-18 5-13 8-15 11-16 13-14 13-15 16-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

13-14

exact bonds :

2-18 5-13 8-15 11-16 13-15 16-17

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

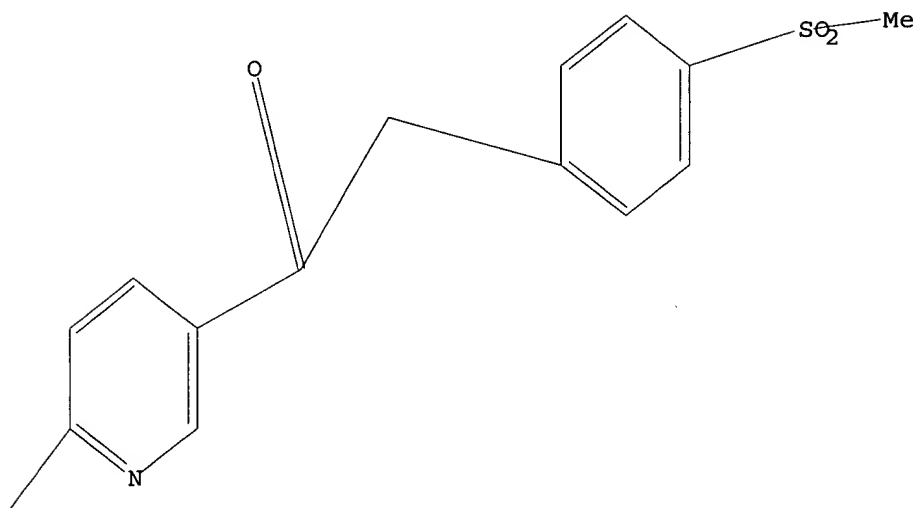
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4 ful

FULL SEARCH INITIATED 15:43:42 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

L5 4 SEA SSS FUL L4

=> d 1-4

L5 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN

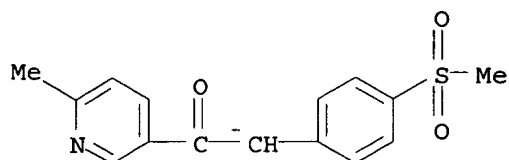
RN 788151-35-9 REGISTRY

ED Entered STN: 25 Nov 2004

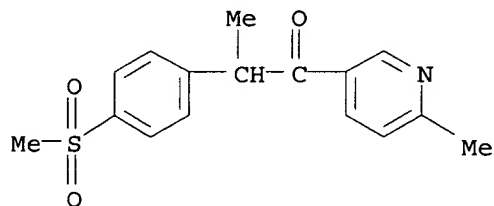
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-)
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H14 N O3 S
 CI COM
 SR CA



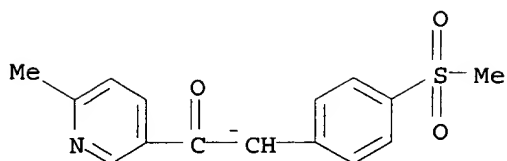
L5 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 452332-13-7 REGISTRY
 ED Entered STN: 18 Sep 2002
 CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C16 H17 N O3 S
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 452332-12-6 REGISTRY
 ED Entered STN: 18 Sep 2002
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-),
 potassium (9CI) (CA INDEX NAME)
 MF C15 H14 N O3 S . K
 SR CA
 LC STN Files: CA, CAPLUS
 CRN (788151-35-9)



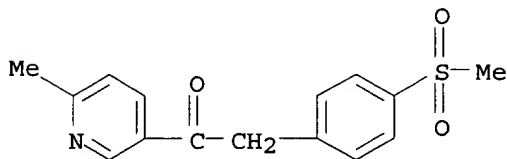
⊖ K⁺

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 221615-75-4 REGISTRY
ED Entered STN: 25 Apr 1999
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
FS 3D CONCORD
MF C15 H15 N O3 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, PS, TOXCENTER, USPAT2,
USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 168.69 | 338.36 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.00 | -0.73 |

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FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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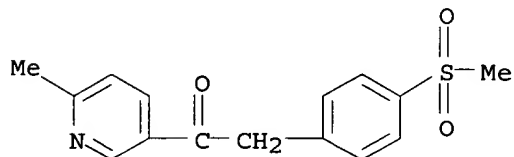
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L6 16 L5

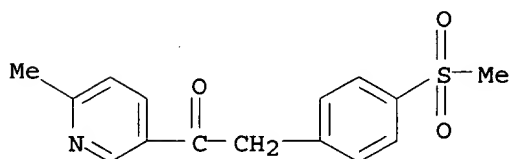
=> d 1-16 fbib abs fhitr

L6 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:406839 CAPLUS
Correction of: 2005:155216
DN 143:248209
Correction of: 142:197768
TI Product class 1: pyridines
AU Spitzner, D.
CS Germany
SO Science of Synthesis (2005), 15, 11-284
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review of methods to prepare pyridines, pyridine-1-oxides, and pyridinium salts. Methods include cyclization, ring transformations, aromatization and substituent modification.
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L6 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:586395 CAPLUS
 DN 140:117549
 TI Development and validation of an HPLC method for the impurity and quantitative analysis of etoricoxib
 AU Hartman, Robert; Abraham, Ahmed; Clausen, Andrew; Mao, Bing; Crocker, Louis S.; Ge, Zhihong
 CS Analytical Research, Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
 SO Journal of Liquid Chromatography & Related Technologies (2003), 26(15), 2551-2566
 CODEN: JLCTFC; ISSN: 1082-6076
 PB Marcel Dekker, Inc.
 DT Journal
 LA English
 AB Etoricoxib (5-chloro-6'-methyl-3[4-(methanesulfonyl)phenyl]-2,3'-bipyridine) is a highly active and selective cyclo-oxygenase II inhibitor. A single, stability-indicating HPLC method was developed and validated for both the impurity and quant. anal. of etoricoxib. Method development incorporated the optimization of stationary phase, pH, temperature, and mobile phase composition for the resolution of 13 process impurities and 3 major degradation products. Further optimization of pH and mobile phase composition was aided by the use of DryLab, a computer-based simulation program. The stability-indicating capability of the method was proven through the identification of photolytic and oxidative decomposition products. Method validation produced excellent results for linearity, precision, limit of quantitation and limit of detection, specificity, accuracy, recovery, and robustness. The identities of etoricoxib decomposition products were confirmed by UV, LC/MS, and NMR spectra.
 IT 221615-75-4
 RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
 (development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)
 RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2003:491189 CAPLUS
 DN 139:70705
 TI Production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of the respective methylthiophenyl derivative
 IN Cannata, Vincenzo; Soriato, Giorgio; Verzini, Massimo
 PA Zambon Group S.P.A., Italy
 SO PCT Int. Appl., 10 pp.
 CODEN: PIXXD2
 DT Patent
 LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|------------|
| PI | WO 2003051843 | A1 | 20030626 | WO 2002-EP14115 | 20021212 |
| | W: CN, CZ, HU, IL, IN, US | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR | | | | |
| | | | | IT 2001-MI2692 | A 20011219 |
| EP | 1492770 | A1 | 20050105 | EP 2002-795165 | 20021212 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK | | | | |
| | | | | IT 2001-MI2692 | A 20011219 |
| | | | | WO 2002-EP14115 | W 20021212 |
| US | 2005165238 | A1 | 20050728 | US 2003-499321 | 20021212 |
| | | | | IT 2001-MI2692 | A 20011219 |
| | | | | WO 2002-EP14115 | W 20021212 |

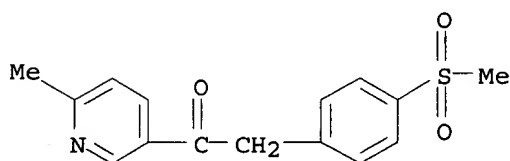
OS CASREACT 139:70705

AB A process for production of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone is carried out by oxidation of 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone with an oxidant in the presence of an acid, the oxidant being a mixture of peracetic acid and hydrogen peroxide, and the acid being methanesulfonic acid. The product is useful as an intermediate in production of cyclooxygenase 2 (COX 2) inhibitors. Thus, the title compound was produced in 88.6% yield by mixing 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone (30), acetic acid (45), methanesulfonic acid (13.6), adding Oxystrong (65% peracetic acid) (28.1 kg) at 35°, and reacting the mixture at 35° for 3-4 h.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:434902 CAPLUS

DN 137:210102

TI Development of a derivatization method, coupled with reverse phase HPLC, for monitoring the formation of an enolate intermediate

AU Abraham, A.; Hartman, R.; Ge, Z.; Mao, B.; Marcoux, J.

CS Merck Research Laboratories, Rahway, NJ, 07065-0914, USA

SO Journal of Liquid Chromatography & Related Technologies (2002), 25(7), 1049-1062

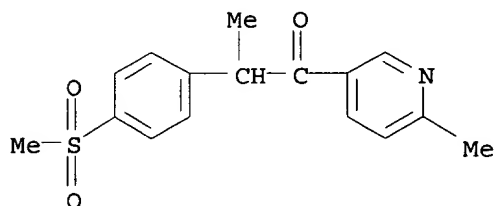
CODEN: JLCTFC; ISSN: 1082-6076

PB Marcel Dekker, Inc.

DT Journal
 LA English
 AB A sensitive liquid chromatog. method was developed to monitor the formation of an enolate intermediate in a synthetic route to Etoricoxib, a drug candidate for the treatment of arthritis. The method requires the derivatization of the enolate with Me iodide to form a stable methylketosulfone derivative followed by reverse phase HPLC anal. Parameters affecting the derivatization, including the nature of derivatizing agent, reaction solvent, amount of derivatizing agent, reaction time, reaction temperature, and amount of excess base in the reaction were studied. The derivatization reaction gave selective C-alkylation. The linear range of the chromatog. method for the determination of the starting material, ketosulfone, and the derivative, methylketosulfone, was determined. Finally, the accuracy of the method was established based on recovery expts.

IT 452332-13-7
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
 (LC-mass spectra of)

RN 452332-13-7 CAPLUS
 CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:276519 CAPLUS
 DN 136:310188
 TI Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound
 IN Heimbrook, David C.; Yao, Siu-long
 PA USA
 SO U.S. Pat. Appl. Publ., 129 pp.
 CODEN: USXXCO

DT Patent
 LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|----------|-----------------------------------|------------------------|
| PI | US 2002042375 | A1 | 20020411 | US 2001-896245 US 2000-216217P | 20010629 P 20000705 |

OS MARPAT 136:310188

AB The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg

= cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given).

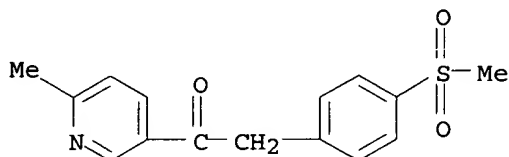
IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L6 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:886073 CAPLUS

DN 136:11103

TI 5-chloro-3-(4-methanesulfonylphenyl)-6'-methyl- [2,3']bipyridinyl in pure crystalline form and process for synthesis

IN Crocker, Louis S.; Davies, Ian W.; Osifchin, Richard G.; Kotliar, Andrew

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|---------------|--|----------|-----------------|------------|
| PI | WO 2001092230 | A1 | 20011206 | WO 2001-US16566 | 20010522 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | CA 2410234 | AA | 20011206 | US 2000-208017P | P 20000526 |
| | | | | CA 2001-2410234 | 20010522 |
| | | | | US 2000-208017P | P 20000526 |
| | | | | WO 2001-US16566 | W 20010522 |
| EP 1296951 | | A1 | 20030402 | EP 2001-939267 | 20010522 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | |
| | | | | US 2000-208017P | P 20000526 |
| | | | | WO 2001-US16566 | W 20010522 |
| JP 2004501116 | | T2 | 20040115 | JP 2002-500844 | 20010522 |
| JP 3665053 | | B2 | 20050629 | | |
| | | | | US 2000-208017P | P 20000526 |
| | | | | WO 2001-US16566 | W 20010522 |
| NZ 522394 | | A | 20040528 | NZ 2001-522394 | 20010522 |

| | | | | | |
|---------------|----|----------|-----------------|----|----------|
| EE 200200655 | A | 20040816 | US 2000-208017P | P | 20000526 |
| | | | WO 2001-US16566 | W | 20010522 |
| | | | EE 2002-655 | | 20010522 |
| | | | US 2000-208017P | P | 20000526 |
| BR 2001011140 | A | 20050111 | WO 2001-US16566 | W | 20010522 |
| | | | BR 2001-11140 | | 20010522 |
| | | | US 2000-208017P | P | 20000526 |
| BG 107237 | A | 20030530 | WO 2001-US16566 | W | 20010522 |
| | | | BG 2002-107237 | | 20021031 |
| | | | US 2000-208017P | P | 20000526 |
| ZA 2002009558 | A | 20031028 | WO 2001-US16566 | W | 20010522 |
| | | | ZA 2002-9558 | | 20021125 |
| | | | US 2000-208017P | P | 20000526 |
| JP 2005047927 | A2 | 20050224 | JP 2004-263913 | | 20040910 |
| | | | US 2000-208017P | P | 20000526 |
| | | | JP 2002-500844 | A3 | 20010522 |

PATENT FAMILY INFORMATION:

FAN 2002:778724

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|-----------------|-------------|
| PI | US 2002147221 | A1 | 20021010 | US 2001-957966 | 20010921 |
| | US 6800647 | B2 | 20041005 | | |
| | | | | US 2000-208017P | P 20000526 |
| | | | | US 2001-865771 | A2 20010525 |
| | US 2002016343 | A1 | 20020207 | US 2001-865771 | 20010525 |
| | US 6521642 | B2 | 20030218 | | |
| | | | | US 2000-208017P | P 20000526 |
| CA 2447878 | AA | 20021205 | CA 2001-2447878 | | 20010921 |
| | | | US 2001-865771 | A | 20010525 |
| | | | WO 2001-US29551 | W | 20010921 |
| WO 2002096877 | A1 | 20021205 | WO 2001-US29551 | | 20010921 |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | | US 2001-865771 | A 20010525 |
| EP 1395562 | A1 | 20040310 | EP 2001-973314 | | 20010921 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| | | | | US 2001-865771 | A 20010525 |
| | | | | WO 2001-US29551 | W 20010921 |
| JP 2004530706 | T2 | 20041007 | JP 2003-500057 | | 20010921 |
| | | | US 2001-865771 | A | 20010525 |
| | | | WO 2001-US29551 | W | 20010921 |
| US 2003153600 | A1 | 20030814 | US 2003-342380 | | 20030114 |
| US 6673935 | B2 | 20040106 | | | |
| | | | US 2001-865771 | A3 | 20010525 |
| JP 2005047927 | A2 | 20050224 | JP 2004-263913 | | 20040910 |
| | | | US 2000-208017P | P | 20000526 |
| | | | JP 2002-500844 | A3 | 20010522 |

AB This invention encompasses the form V polymorph of the title composition which is useful in the treatment of cyclooxygenase-2 mediated diseases. The invention encompasses certain pharmaceutical compns. for treatment of cyclooxygenase-2 mediated diseases comprising the Form V polymorph of the title composition The invention also encompasses a process for synthesizing

the form V polymorph of the title composition A mixture of the title composition and iso-Pr acetate was heated at 55°, then was cooled to ambient temperature and the solids were isolated by filtration. The solids were washed with iso-Pr acetate and dried in vacuo to give the form V polymorph as a colorless solid in about 87% yield.

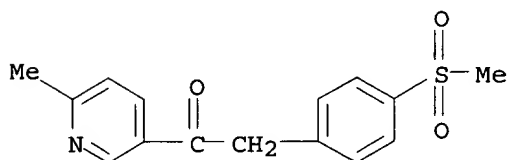
IT 221615-75-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300685 CAPLUS

DN 134:311114

TI Process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone

IN Cannata, Vincenzo; Rossato, Roberto

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 9 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2001029004 | A1 | 20010426 | WO 2000-EP9995 | 20001011 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| IT 99MI2156 | A1 | 20010416 | IT 1999-MI2156 | 19991015 |
| CASREACT 134:311114 | | | IT 1999-MI2156 | 19991015 |
| AB A process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone (I) into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone, a pharmaceutical intermediate (no data), without the formation of N-oxide byproduct, consists of reacting I with an oxidant (e.g., a mixture of peracetic acid and hydrogen peroxide) in the presence of a catalyst (e.g., sodium tungstate) and an acid (e.g. | | | | |

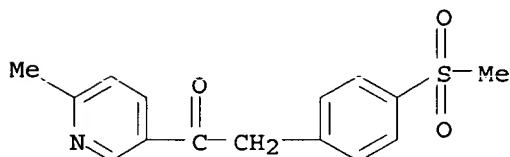
methanesulfonic acid).

IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300684 CAPLUS

DN 134:295751

TI Process for the preparation of intermediates useful in the synthesis of diarylpyridines

IN Allegrini, Pietro; Verzini, Massimo

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 20 pp.
 CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2001029003 | A1 | 20010426 | WO 2000-EP9994 | 20001011 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| IT 99MI2157 | A1 | 20010416 | IT 1999-MI2157 | 19991015 |
| | | | IT 1999-MI2157 | 19991015 |

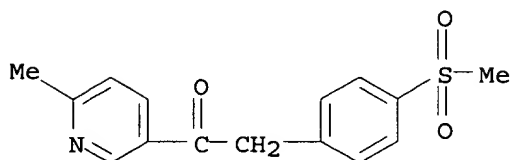
OS CASREACT 134:295751; MARPAT 134:295751

AB This process is used to prepare intermediates useful in the synthesis of diarylpyridines having COX-2 inhibitor activity. E.g., reaction of 6-methylnicotinic acid Me ester with (4-methylthiophenyl)acetonitrile gave 3-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)-3-oxopropionitrile hydrochloride. Acid hydrolysis and decarboxylation of the latter gave 1-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)ethanone.

IT 221615-75-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the preparation of intermediates useful in the synthesis of diarylpyridines)

RN 221615-75-4 CAPLUS
 CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)

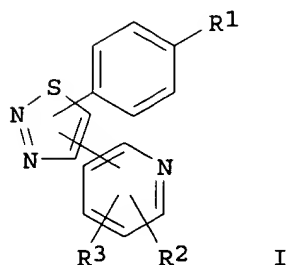


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2001:185752 CAPLUS
 DN 134:222716
 TI 1,2,3-Thiadiazoles and their use as COX-2 inhibitors
 IN Lau, Cheuk K.; Li, Chun Sing; Therien, Michel; Gauthier, Jacques Y.
 PA Merck Frosst Canada & Co., Can.
 SO PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2001017996 | A1 | 20010315 | WO 2000-CA1040 | 20000907 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 1999-152746P P 19990908 | | | | |

OS MARPAT 134:222716
 GI



AB Title compds. I [R1 = SO₂Me, S(O)NHMe, S(O)NHNH₂, P(O)MeOH, etc.; R2, R3 = H, halo, alkoxy, alkyl, CN, etc.] were prepared Thus, 4-(6-methyl-3-pyridinyl)-5-[4-(methylsulfonyl)phenyl]-1,2,3-thiadiazole (II) was prepared

in 5 steps starting from 6-methylnicotinic acid and N-methoxymethylamine hydrochloride. Oxidation of II with H₂O₂ gave the thiadiazole 3-oxide. Inhibition of COX-2 was determined by measuring the effects on PGE₂ production

in

whole blood.

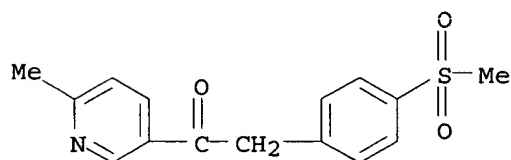
IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:78362 CAPLUS

DN 134:131435

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone starting from 4-methylthiobenzyl alcohol and 6-methylnicotinate esters.

IN Bessard, Yves; Leresche, James Edward

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2001007410 | A1 | 20010201 | WO 2000-EP6825 | 20000717 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | EP 1999-114667 | A 19990727 |
| | | | US 2000-186680P | P 20000303 |
| EP 1198455 | A1 | 20020424 | EP 2000-951393 | 20000717 |
| EP 1198455 | B1 | 20031210 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | | | EP 1999-114667 | A 19990727 |
| | | | US 2000-186680P | P 20000303 |
| | | | WO 2000-EP6825 | W 20000717 |
| JP 2003505449 | T2 | 20030212 | JP 2001-512497 | 20000717 |

| | | | | | |
|---------------|----|----------|-----------------|----|----------|
| | | | EP 1999-114667 | A | 19990727 |
| | | | US 2000-186680P | P | 20000303 |
| | | | WO 2000-EP6825 | W | 20000717 |
| AT 256112 | E | 20031215 | AT 2000-951393 | | 20000717 |
| | | | EP 1999-114667 | A | 19990727 |
| | | | US 2000-186680P | P | 20000303 |
| | | | WO 2000-EP6825 | W | 20000717 |
| ES 2207536 | T3 | 20040601 | ES 2000-951393 | | 20000717 |
| | | | EP 1999-114667 | A | 19990727 |
| | | | US 2000-186680P | P | 20000303 |
| US 6566527 | B1 | 20030520 | US 2002-30096 | | 20020314 |
| | | | EP 1999-114667 | A | 19990727 |
| | | | US 2000-186680P | P | 20000303 |
| | | | WO 2000-EP6825 | W | 20000717 |
| US 2003088107 | A1 | 20030508 | US 2002-283167 | | 20021030 |
| US 6600046 | B2 | 20030729 | | | |
| | | | EP 1999-114667 | A | 19990727 |
| | | | US 2000-186680P | P | 20000303 |
| | | | WO 2000-EP6825 | W | 20000717 |
| | | | US 2002-30096 | A3 | 20020314 |

OS CASREACT 134:131435

AB 1-(6-Methylpyridin-3-yl)-2-[(4-methylsulfonyl)phenyl]ethanone was prepared by (a) treatment of 4-(methylthio)benzyl alc. with hydrochloric acid to give 4-(methylthio)benzyl chloride, (b) treatment of this with an alkali metal cyanide to give 4-(methylthio)phenylacetonitrile, (c) condensation of 4-(methylthio)phenylacetonitrile with a 6-methylnicotinate ester to give 3-[2-(4-methylthiophenyl)-2-cyanoacetyl]-6-methylpyridine, (d) hydrolysis and decarboxylation under acidic conditions to give 3-[2-(4-methylthiophenyl)acetyl]-6-methylpyridine and (e) oxidation

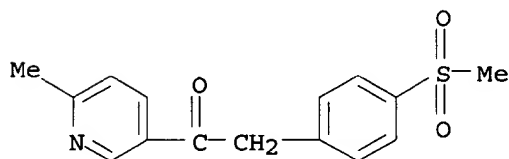
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl)ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:897114 CAPLUS

DN 134:178439

TI A general [3 + 2 + 1] annulation strategy for the preparation of pyridine N-oxides

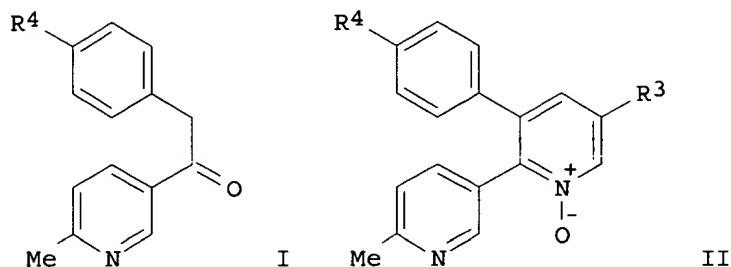
AU Davies, Ian W.; Marcoux, Jean-Francois; Reider, Paul J.

CS Department of Process Research, Merck & Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2001), 3(2), 209-211

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 134:178439
 GI

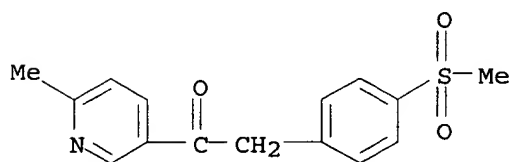


AB Stabilized ketone, aldehyde, and ester enolates, generated from I ($R_4 = \text{MeSO}_2, \text{MeS}$) for example, react with vinamidinium hexafluorophosphate salts and hydroxylamine hydrochloride to give pyridine N-oxides, e.g. II ($R_3 = \text{Cl}, \text{NO}_2$), in 45-85% yields.

IT 221615-75-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

RN 221615-75-4 CAPLUS

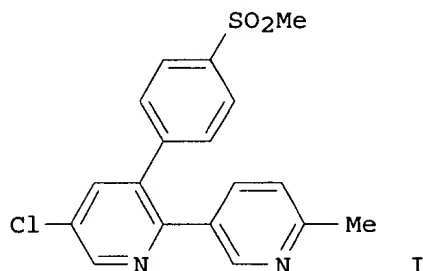
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:653182 CAPLUS
 DN 134:4838
 TI A Practical Synthesis of a COX-2-Specific Inhibitor
 AU Davies, Ian W.; Marcoux, Jean-Francois; Corley, Edward G.; Journet, Michel; Cai, Dong-Wei; Palucki, Michael; Wu, Jimmy; Larsen, Robert D.; Rossen, Kai; Pye, Philip J.; DiMichele, Lisa; Dormer, Peter; Reider, Paul J.
 CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA
 SO Journal of Organic Chemistry (2000), 65(25), 8415-8420
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English

OS CASREACT 134:4838
GI



AB A number of synthetic strategies to the Cox-2 specific inhibitor have been described. These studies have led to the identification of a novel pyridine construction using annulation of a ketone using a vinamidinium species and ammonia in 97% assay yield. Three approaches to the synthesis of the ketone are described that allow for its preparation in large quantities in >65% overall yield from Me 6-methylnicotinate.

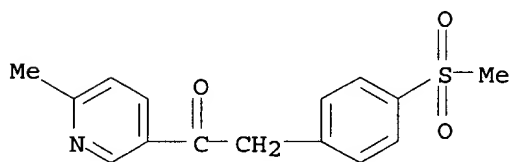
IT 221615-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:493518 CAPLUS

DN 133:104966

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.

IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 19 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|------|----------|-----------------|----------|
| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |
| | WO 2000042014 | A3 | 20001207 | | |

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---------------|--|----------|-----------------|----|----------|
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| CA 2359958 | AA | 20000720 | CA 2000-2359958 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| CA 2485739 | AA | 20000720 | CA 2000-2485739 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | CA 2000-2359958 | A3 | 20000113 |
| EP 1159270 | A2 | 20011205 | EP 2000-901555 | | 20000113 |
| EP 1159270 | B1 | 20031105 | | | |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| JP 2003518002 | T2 | 20030603 | JP 2000-593582 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| AT 253559 | E | 20031115 | AT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| EP 1394149 | A1 | 20040303 | EP 2003-24787 | | 20000113 |
| EP 1394149 | B1 | 20050119 | | | |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |
| | | | EP 1999-100590 | A | 19990114 |
| | | | EP 2000-901555 | A3 | 20000113 |
| PT 1159270 | T | 20040331 | PT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| ES 2209807 | T3 | 20040701 | ES 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| AT 287396 | E | 20050215 | AT 2003-24787 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| PT 1394149 | T | 20050531 | PT 2003-24787 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| ES 2235138 | T3 | 20050701 | ES 2003-3024787 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | WO 2000-EP240 | W | 20000113 |
| NO 2001003498 | A | 20010905 | NO 2001-3498 | | 20010713 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| US 2005159458 | A1 | 20050721 | US 2005-29489 | | 20050106 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |

WO 2000-EP240
US 2003-868941

W 20000113
A3 20031104

OS CASREACT 133:104966

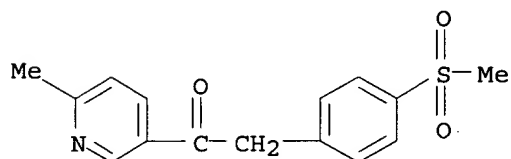
AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared. Thus, N,N-diethylamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L6 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:443023 CAPLUS

DN 133:222553

TI Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines

AU Marcoux, Jean-Francois; Corley, Edward G.; Rossen, Kai; Pye, Phil; Wu, Jimmy; Robbins, Michael A.; Davies, Ian W.; Larsen, Robert D.; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2000), 2(15), 2339-2341

CODEN: ORLEF7; ISSN: 1523-7060

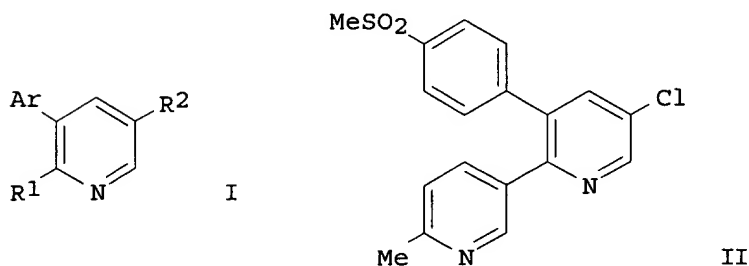
PB American Chemical Society

DT Journal

LA English

OS CASREACT 133:222553

GI

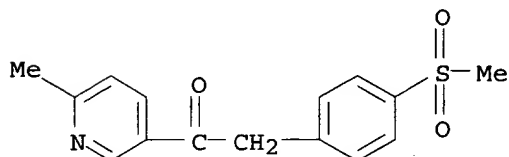


AB α -Aryl ketones react with vinamidinium hexafluorophosphate salts to give access to the corresponding 3-arylpyridines I (Ar = C₆H₄R-4, R = SO₂Me, H, SMe, R₁ = 6-methyl-3-pyridyl, C₆H₄R-4, R₂ = Cl; Ar = C₆H₄SO₂Me-4, R₁ = 6-methyl-3-pyridyl, R₂ = Br, I, CF₃, NO₂, phthalimido; Ar = C₆H₄F-4, R₁ = Me, R₂ = Cl; Ar = Ph, R₁ = H, R₂ = Cl). The annulation reactions proceed in good to excellent yields with vinamidinium salts containing electron-withdrawing groups at the β -position (R₂). The reaction was applied to the preparation of the COX-2 specific inhibitor 5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine (II), as well as a series of analogs.

IT 221615-75-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

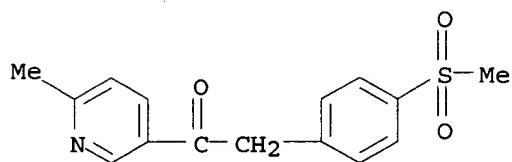
L6 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:708874 CAPLUS
 DN 131:322542
 TI Process for synthesizing arylpyridine COX-2 inhibitors
 IN Corley, Edward G.; Davies, Ian W.; Larsen, Robert D.; Pye, Philip J.;
 Rossen, Kai
 PA Merck & Co., Inc., USA
 SO PCT Int. Appl., 29 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|--|----------|-----------------|------------|
| WO 9955830 | A2 | 19991104 | WO 1999-US8645 | 19990420 |
| WO 9955830 | A3 | 19991229 | | |
| W: | AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| CA 2329193 | AA | 19991104 | CA 1999-2329193 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |

| | | | | |
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| EP 1071745 | A2 | 20010131 | EP 1999-918706 | 19990420 |
| EP 1071745 | B1 | 20040804 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO | | | | |
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| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| BR 9909844 | A | 20010403 | BR 1999-9844 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| JP 2002513035 | T2 | 20020508 | JP 2000-545976 | 19990420 |
| JP 3325264 | B2 | 20020917 | | |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| AU 759469 | B2 | 20030417 | AU 1999-36557 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| CZ 292515 | B6 | 20031015 | CZ 2000-3940 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| NZ 507597 | A | 20040227 | NZ 1999-507597 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| AT 272613 | E | 20040815 | AT 1999-918706 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| PT 1071745 | T | 20041130 | PT 1999-918706 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| ES 2226378 | T3 | 20050316 | ES 1999-918706 | 19990420 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| US 6040319 | A | 20000321 | US 1999-298127 | 19990423 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| TW 474934 | B | 20020201 | TW 1999-88106545 | 19990423 |
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| | | | US 1998-85668P | P 19980515 |
| US 6252116 | B1 | 20010626 | US 2000-488774 | 20000121 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | US 1999-298127 | A3 19990423 |
| HR 2000000722 | A1 | 20010630 | HR 2000-722 | 20001024 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | W 19990420 |
| HK 1031399 | A1 | 20041217 | HK 2001-102195 | 20010326 |
| | | | US 1998-82888P | P 19980424 |
| | | | US 1998-85668P | P 19980515 |
| | | | WO 1999-US8645 | A 19990420 |
| OS | CASREACT 131:322542; MARPAT 131:322542 | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB The invention encompasses a process and intermediates for preparing compds. I [R, R', R'' = (un)substituted alkyl, aryl, aralkyl, halo, SOMH, SOM-alkyl, SOM-aryl, NO₂, (di)(alkyl)amino, SOMNH₂, SOMNH-alkyl, SOMNHCOCF₃, cyano; Y = C, N; m = 0, 1, 2]. I are useful in the treatment of cyclooxygenase-2 mediated diseases (no data), i.e., as analgesics, antipyretics, and antiinflammatories. The method comprises cyclocondensation of an iminium salt II [R₂-R₅ = alkyl, aryl, or aralkyl; X- = suitable counterion] with an aryl ketone III in the presence of a base. The method is designed to give high yields at low temps., and with a reduced number of steps. For instance, the bipyridyl derivative IV was prepared on a 1.65-kg scale by reaction of the iminium salt V with ketone VI in THF in the presence of KOBu-tert, followed by quenching in AcOH/THF, basification with concentrated aqueous NH₄OH, and refluxing. Prepns. of the salt and ketone intermediates V and VI are described, and a subset of the iminium salt intermediates II are claimed per se.
- IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)
- RN 221615-75-4 CAPLUS
- CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
 (CA INDEX NAME)



L6 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:222917 CAPLUS
 DN 130:252250
 TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.
 IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
 PA Merck & Co., Inc., USA
 SO PCT Int. Appl., 42 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----|--|------|----------|-----------------|----------|
| PI | WO 9915503 | A2 | 19990401 | WO 1998-US19788 | 19980922 |
| | WO 9915503 | A3 | 19990520 | | |
| W: | AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: | GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, | | | | |

CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|----|----------|-----------------|----|----------|
| | | | US 1997-60680P | P | 19970925 |
| | | | GB 1998-6419 | A | 19980325 |
| US 6040450 | A | 20000321 | US 1998-153405 | | 19980915 |
| | | | US 1997-60680P | P | 19970925 |
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| EP 1023266 | A2 | 20000802 | EP 1998-948426 | | 19980922 |
| EP 1023266 | B1 | 20030108 | | | |
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| | | | GB 1998-6419 | A | 19980325 |
| | | | WO 1998-US19788 | W | 19980922 |

OS CASREACT 130:252250; MARPAT 130:252250

AB P-(ArCOCH₂)C₆H₄SO₂R₁ (R₁ = Me, NH₂, NHCOCF₃, NHMe; Ar = mono-, di-, or trisubstituted Ph, pyridyl, N-oxide thereof), were prepared by reaction of p-MeSC₆H₄CH₂MgX (X = Cl, Br, F, iodo) with ArCONMe₂ (Ar as above) to give p-(ArCOCH₂)C₆H₄SMe followed by oxidation of the latter. Thus, the Grignard reagent from p-MeSC₆H₄CH₂Cl in PhMe/THF was added to a -20° solution of 6-methylnicotinic acid N-methyl-N-methoxyamide (preparation given) in PhMe over 30 min. followed by 1 h aging to give 76% 2-methyl-5-(4-methylthiophenylacetyl)pyridine. The latter in MeOH/H₂SO₄ at 55° was treated with aqueous Na tungstate and then with H₂O₂ over 1 h to give 82.5% 2-methyl-5-(4-methylsulfonylphenylacetyl)pyridine. The latter

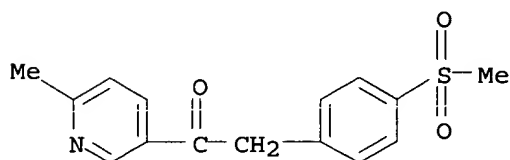
reacted with 3-amino-2-chloroacrolein (preparation given) to give 65%
5-chloro-2-(2-methylpyrid-5-yl)-3-(4-methylsulfonylphenyl)pyridine.

IT 221615-75-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



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Executing the logoff script...

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TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

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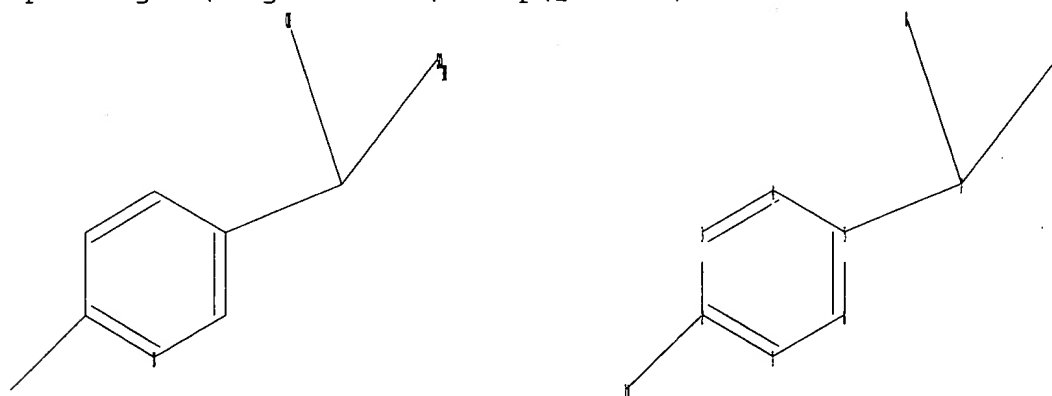
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7 8 9 10

ring nodes :

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chain bonds :
2-10  5-7  7-8  7-9
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
7-8
exact bonds :
2-10  5-7  7-9
normalized bonds :
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isolated ring systems :
containing 1 :

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Match level :

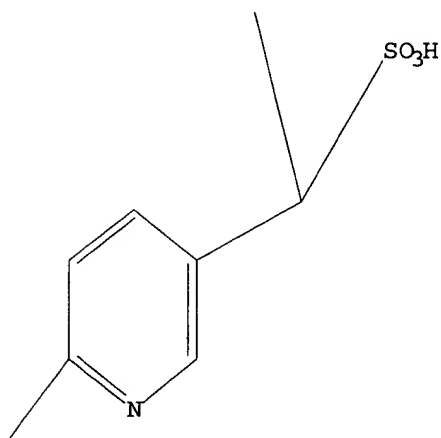
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L1 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 32 TO ITERATE

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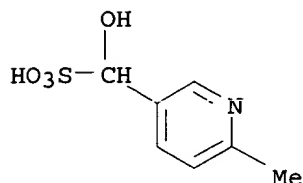
2 ANSWERS

SEARCH TIME: 00.00.01

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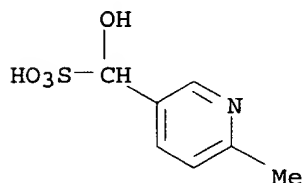
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L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 763071-57-4 REGISTRY
 ED Entered STN: 15 Oct 2004
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 FS 3D CONCORD
 MF C7 H9 N O4 S
 CI COM
 SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 283167-58-8 REGISTRY
 ED Entered STN: 04 Aug 2000
 CN 3-Pyridinemethanesulfonic acid, α -hydroxy-6-methyl-, monosodium salt (9CI) (CA INDEX NAME)
 MF C7 H9 N O4 S . Na
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 CRN (763071-57-4)



● Na

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

| SINCE FILE | TOTAL |
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| ENTRY | SESSION |
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FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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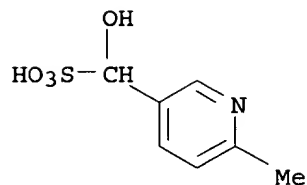
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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethane.
IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |
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| | RW: | | | | |
| | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
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| AT 253559 | E | 20031115 | AT 2000-901555 | 20000113 |
| | | | EP 1999-100590 | A 19990114 |
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| | | | US 2003-868941 | A3 20031104 |
| OS | CASREACT 133:104966 | | | |
| AB | 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared. Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I. | | | |
| IT | 283167-58-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone) | | | |
| RN | 283167-58-8 CAPLUS | | | |
| CN | 3-Pyridinemethanesulfonic acid, α -hydroxy-6-methyl-, monosodium salt | | | |

(9CI) (CA INDEX NAME)



● Na

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L3 1 S L2

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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